MATHEMATICAL THEORY OF SCATTERING IN QUANTUM MECHANICS—A REVIEW

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ABSTRACT

A brief review of the mathematical theory of quantum mechanical scattering is given from the time-dependent point of view, Some of the proofs for completeness in the 2-body case are discussed.

NEARLY thirty years have passed since the foundation of the mathematical theory of scattering in quantum mechanics was laid by Jauch[1] and Cook[2]. Significant advances have been achieved in these thirty years mainly in the domain of time-independent theory due to the pioneering works of Kato, Kuroda, Agmon and others. These methods have been extensively discussed in the books [AJS[3]], [RS[4] Vols. III and IV] and [Sigal[5]]. All these theories essentially study the resolvent operator $(H-Z)^{-1}$ of the relevant Hamiltonian H as $Z\to\lambda\pm io$ where λ belongs to the spectrum of H, and involves a careful analysis of the Green's function near the spectrum of H. These methods should more appropriately be called the spectral analysis of the continuous part of H. Recently Enss[6] initiated a direct time-dependent method which relies on the time description of the physical phenomenon of scattering. Now one has very satisfactory theories of 2-, 3- and 4- body scattering, short as well as long-range, mainly due to the efforts of Enss[6], Mourre[7], Perry[8] and also our group at the Indian Statistical Institute[9-11]. Very recently Sigal and Soffer[12] have given a proof for N-body case. We shall briefly outline this second line of developments.

We start with the Dirac-von Neumann description of quantum mechanics viz that we have a Hilbert space $\mathscr{H}$ as a receptacle of the quantum mechanical system with the states of the system being given by the vectors (unit rays to be more precise) in $\mathscr{H}$ and the observables by some suitable subset of the self adjoint operators in $\mathscr{H}$. The dynamical evolution of the system is then given by a one-parameter group of unitary operators in $\mathscr{H}$, whose self-adjoint infinitesimal generator H is called the Hamiltonian of the system. A physical system is characterized by the choice of the kinematical variables, say position $\mathbf{Q}$ and momentum $\mathbf{P}$ observables, and then a certain Hamiltonian H is constructed as a function of these observables.

More specifically, for a system of N indistinguishable particles without spin and moving non-relativistically, the appropriate Hilbert space is $\mathscr{H}\equiv L^2(\mathrm{R}^{3N})$, consisting of (equivalent classes of) complex square-integrable functions of N 3-vector variables, and the positions $\mathbf{Q}_i$ and momenta $P_i (i=l,\ldots N)$ observables are given as

$$(\mathbf{Q}_j f)(\mathbf{X}_l,\ldots,\mathbf{X}_N)=\mathbf{X}_j f(\mathbf{X}_l,\ldots,\mathbf{X}_N),$$
$$(\mathbf{P}_j f)(\mathbf{X}_l,\ldots,\mathbf{X}_N)=-i\nabla_j f(\mathbf{X}_l,\ldots,\mathbf{X}_N),$$

with natural domains (we have put $\hbar=1$ for convenience). Note that $\mathbf{Q}_j$'s are all self-adjoint while $\mathbf{P}_j$'s are not a 'natural' self-adjoint extension can be obtained by using the L^2 theory of Fourier transform (see reference 3) which are also denoted by $\mathbf{P}_j$. For a non-relativistic situation, a typical (Galilean covariant) Hamiltonian H is given as

$$H=H_o+V\equiv H_o+\sum_{j<k}V_{jk}(x_j-x_k), \qquad (2)$$

where $H_o=\sum_j(2m_j)^{-1}\mathbf{P}_j^2$ and V_{jk}'s are pair potentials. A transformation to the centre of mass coordinate system reduces the above to

$$H=H_{cM}+H_{rel}=H_{cM}+(\sum(2\mu_j)^{-1}\mathbf{P}_j^2+\sum V_{jk}),$$

in the decomposition

$$\mathscr{H} = L^2_{cM}(\mathrm{R}^3) \otimes L^2(\mathrm{R}^{3(N-1)}),$$

where $\mathbf{P}_j$ are the relative momenta in the Jacobi coordinate system. The potentials are called short-range if $|V_{jk}(x)| \sim |x|^{-1-\delta}$, $\delta > 0$ as $|x| \to \infty$ for every j, k, otherwise it is long-range.

The first problem is to prove that H or H_{rel} is self-adjoint and this is achieved for a large class of potentials by using the calebrated Rellich-Kato theorem. This is done by showing directly that H_o is self-adjoint and then proving that $\sum V_{jk}$ is 'very small' relative to H_o. Details can be found in references 3 and 4.

Once we have a self-adjoint H, we write the total Schrödinger evolution group $V_t \equiv \exp(-iHt)$ and ask the first question of scattering theory: what is the asymptotic behaviour of V_t in the distant past and remote future? Since $\mathscr{H}$ is ∞-dimensional, the concept of proximity between states is not fixed and there are many possibilities. However a careful study shows[3] that in most cases the natural metric of $\mathscr{H}$ is enough. Intuitively it is clear that if the interaction potentials decay to O at ∞ 'sufficiently fast', then V_t should asymptotically look like any of the possibilities described below.

Let D be a partition of $\{1,2,\ldots,N\}$ into $n(\geq 2)$ clusters (1), (2), ..., (n). The associated cluster Hamiltonian H^D is obtained from H by dropping in V all interactions between particles in different clusters i.e.

$$H^D = H_o + \sum_{k=1}^{n} \sum_{i<j\in(k)} V_{ij}. \quad (3)$$

Then it follows that H^D is also self-adjoint on $D(H_o)$ and we write $U_t^D \equiv \exp(-itH^D)$ for the evolution of the clustering D. Intuitively it appears that for large negative and positive times the total evolution V_t looks like U_t^D for some D. In particular, one possibility is that all N particles are free i.e. a partition D with $n = N$ and cluster Hamiltonian H_o. Thus the first problem of scattering theory is to establish this for some class of pair potentials. The next theorem gives a typical result in this direction, the proof of which can be found in reference 3.

Theorem 1: Assume that each pair potential V_{jk} belongs to $L^2(\mathbf{R}^3)$. Then (i) the wave operators $\Omega^D_\pm \equiv s-\lim V_t^* U_t^D$ as $t \to \pm\infty$ exist, (ii) $H\Omega^D_\pm = \Omega^D_\pm H^D$, the intertwining property is satisfied, (iii) setting $F^D_\pm \equiv \Omega^D_\pm \Omega^{D*}_\pm$, the orthogonal projection onto the ranges of the isometries $\Omega^D_\pm$, one has furthermore $F^c_\pm F^D_\pm = \delta_{cD} F^D_\pm$.

The conclusion (i) implies that for every state of the form $\Omega^D_\pm f$ under the total evolution V_t 'looks like' $U_t^D f$ at distant past ($-$ve sign) and at remote future ($+$ve sign) respectively. The second result means that H restricted to the reducing subspaces $F^D_\pm$ are unitarily equivalent to the absolutely continuous operator H^D. The implication of (iii) is that the subspace of the vectors of the form $\Omega^D_\pm f$ is orthogonal to the one of the form $\Omega^c_\pm g$ when C and D are distinct clusterings. Let us now add up (precisely, take direct sums) of these orthogonal subspaces i.e. write $F_\pm = \sum_D F^D_\pm$. Since we believe that all possible asymptotic states have been counted, this sum should give all the scattering states, and also we do not expect any asymmetry between past and future leading to our writing $F_+ = F_- = I - P_b$, where P_b is the projection onto the N-body bound states. This is the second (and much more difficult than the first one) problem of scattering theory and is often known as the problem of N-body asymptotic completeness. It is not possible here to even begin to describe some of these methods in detail and we shall only deal briefly with the simpler case when $N = 2$. But before that we say a few words about this problem itself, confining ourselves to $N = 2$ case for simplicity.

If we define the scattering operator $S = \Omega^*_+ \Omega_-$, then for the definition of S we need only that the range of Ω_- is contained in that of Ω_+, i.e. $F_- \leq F_+$. However in such a case, S is only isometric and S is unitary if and only if $F_- = F_+$. Contrary to what one may think, the existence of an anti-unitary time-reversal symmetry (since H is a real operator!) has no bearing on the problem unless one has already managed to show that $F_- \leqslant F_+$. In practice, one directly shows the equality without bringing time-reversal into consideration. In fact one can construct examples of real Hamiltonians with potentials of compact support, but very singular near the origin and also oscillatory with the period decreasing as one approaches the origin such that the projections F_+ and F_- are not comparable though the wave operators exist. In such a model, a part of the incoming wave gets absorbed in the scattering centre and the rest gets scattered while a part of the outgoing wave is created from the scattering centre and the rest appears to have come from some incoming projectile. In this model, S is not unitary, not even isometric. The details of such bizarre yet interesting situation can be found in (references 3 and 13).

Now we briefly describe the proof of the asymptotic completeness for the 2-body short-range problem by the time-dependent method. In this version the generator of the dilation group plays an important role. In $\mathscr{H} = L^2(\mathbf{R}^3)$, set

$$(Y_\theta f)(x) = \exp(-3\theta/4) f[\exp(-\theta/2)x] \quad \forall f \in \mathscr{H},\ \theta \in \mathbf{R}. \tag{4}$$

so that Y_θ is a unitary strongly continuous representation of the dilation group in $\mathbf{R}^3$ with its generator

$$A = \tfrac{1}{4}(P.Q + Q.P) \text{ on } \rho(\mathbf{R}^3).$$

One then easily verifies the commutation rules:

$$[A, \mathbf{P}] = \tfrac{i}{2}\mathbf{P}, [A, \mathbf{Q}] = -\tfrac{i}{2}\mathbf{Q}, [A, H_o] = iH_o. \tag{5}$$

Here $H_o = \frac{1}{2}\mathbf{P}^2$, the relative free Hamiltonian in the cM system with relative mass $\mu = 1$. The last relation in (5) can be rewritten as $[A, \ln H_o] = i$ which is just like the relation $[q, p] = i$ in $1-D$ quantum mechanics. However, caution is to be exercised due to the fact that since both A and $\ln H_o$ are rotationally invariant, they have an underlying degeneracy space which is just the L^2 of the unit sphere in $\mathbf{R}^3$. The commutation relations (5) also tell us that the self-adjoint operator A with the whole $\mathbf{R}$ as its (absolutely) continuous spectrum 'behaves much like Q' which will be made precise in the next lemmas.

Lemma 2: $(1+|Q|)^{-\alpha}(H_o+1)^{-1}(1+|A|)^{\alpha}$ is a bounded operator in $\mathscr{H}$ for all α such that $0 \leqslant \alpha \leqslant 2$. Proof is by first observing that the conclusion is true for $\alpha = 0, 2$ by (5) and then applying interpolation (see reference 4).

Lemma 3: Let $P_\mp \; P(|A| < \kappa|t|)$ denote the projections corresponding to the spectral sets $A \lessgtr 0, |A| < \kappa|t|$ respectively, and let ϕ be a C^∞ function of compact support in $\mathbf{R}^+ - \{o\}$ with $2\kappa = \inf \operatorname{supp} \phi$. Also assume that the 2-body potential V is such that $V(H_o+1)^{-1}(1+|Q|)^{1+\delta}$ is compact for some $\delta > 0$ (e.g. if $(1+|Q|)^{1+\delta} V \in L^\infty(\mathbf{R}^3) + L^2(\mathbf{R}^3)$). Then

(i) $\|P(|A| < \kappa|t|)\exp(-iH_o t)\phi(H_o)P_\pm\| \leqslant C_N(1+|t|)^{-N}$ for $t \lessgtr 0$

respectively and for every positive integer N,

(ii) $\|V\exp(-iH_o t)\phi(H_o)P_\pm\| \leqslant C_N(1+|t|)^{-1-\delta}$ for $t \lessgtr 0$,

(iii) $[\phi(H) - \phi(H_o)]$ and $(\Omega_\pm - 1)\phi(H_o)P_\pm$ are compact operators in $\mathscr{H}$,

(iv) $\text{s}-\lim P_\pm \exp(-iH_o t)\phi(H_o) = 0$ as $t \to \mp\infty$.

Sketch of proof (for $t > 0$): i) From (5) it follows that $\exp(iH_o t) A \exp(-iH_o t) = A + H_o t$ and therefore $\phi(H_o)\exp(-iH_o t) P_+ \exp(iH_o t) = \phi(H_o)P(A > H_o t)$ implies classically a region where $A > 2\kappa t$ which is disjoint from $|A| < \kappa|t|$. The inverse power decay comes from the quantum overlap of two classically disjoint regions and exact estimates can be obtained using the method of stationary phase (see reference 10).

(ii) $\|(1+|A|)^{-\alpha}\exp(-iH_o t)\phi(H_o)P_\pm\| \leqslant \|(1+|A|)^{-\alpha}P(|A| > \kappa|t|)\| + \|P(|A| < \kappa|t|)\exp(-iH_o t)\phi(H_o)P_\pm\| \leqslant C(1+|t|)^{-\alpha}$ by (i).

On the other hand, writing

$$V\exp(-iH_o t)\phi(H_o)P_\pm = \{V(H_o+1)^{-1}(1+|Q|)^{1+\delta}\}\{(1+|Q|)^{-1-\delta}(H_o+1)^{-1}(1+|A|)^{1+\delta}\}.$$

$\{(1+|A|)^{-1-\delta}\exp(-iH_o t)\phi(H_o)P_\pm\}$ and observing that the first two terms are bounded by hypothesis and Lemma 2 respectively, we have the result on applying (i) to the last part.

(iii) Firstly, we note that $\phi(H)-\phi(H_o)$ is compact just as $(H+i)^{-1}-(H_o+i)^{-1}=-(H+i)^{-1}V(H_o+i)$ is compact by hypothesis. That $(\Omega_\pm-1)\phi(H_o)P_\pm$ are compact follows by writing the expression $(\Omega_+-1)\phi(H_o)P_+=i\int_o^\infty \exp(iHt)V\phi(H_o)\exp(-iH_o t)P_+$ and observing that the integrand is compact by hypothesis while the integral converges in norm by (ii).

(iv) From the proof of (ii) we have that

$$\|P_\pm \exp(\pm iH_o t)\phi(H_o)(1+|A|)^{-\alpha}\|=\|(1+|A|)^{-\alpha}\exp(\mp iH_o t)\phi(H_o)P_\pm\|$$

$\to 0$ as $t\to\pm\infty$ and the required result follows by observing that the range of $(1+|A|)^{-\alpha}$ is dense.

Theorem 4: Let v be as in Lemma 3. Then the scattering system is asymptotically complete.

Proof: We shall show that $F_+=E_c(H)$, the projection onto the continuous part of H. Since the proof is symmetric w.r.t. the sign, this implies that $F_+=F_-=E_c(H)$.

By Theorem 1 (ii), $F_+\leqslant E_c(H)$ and we set $F'_+=E_c(H)-F_+$ which we assume to be non-zero. Since both F_+ and $E_c(H)$ reduce H, so does F'_+ and since the continuous spectrum of H is $\mathbf{R}^+$, a dense set in F'_+ is given by $\mathcal{D}_+=\{\phi(H)f|f\in F'_+\mathscr{H},\ \phi$ compact support in $\mathbf{R}^+-\{0\}\}$. Thus we restrict our attention to vectors with total energy support compact in $\mathbf{R}^+-\{0\}$ i.e. $f\in F'_+\mathscr{H}$, $f=\phi(H)f$ and show that this leads to a contradiction unless $f=0$.

We set $\varepsilon_\pm(\xi(t))=\lim \pm T^{-1}\int_o^{\pm T}\xi(t)\,dt$, where ξ is a bounded continuous function and note after Wiener (see reference 3) that if B is compact and if $f\in E_c(H)\mathscr{H}$, then $\varepsilon_\pm(\|B\exp(-iHt)f\|)=0$. Thus

$$\|f\|^2=\varepsilon_+(\|\exp(-iHt)f\|^2)=\varepsilon_+((\exp(-iHt)f,\ \phi(H)\exp(-iHt)f))=\varepsilon_+((\exp(-iHt)f,\ \Omega_+\phi(H_o)P_+\exp(-iHt)f))-$$
$$\varepsilon_+((\exp(-iHt)f,(\Omega_+-1)\phi(H_o)P_+\exp(-iHt)f))+$$
$$\varepsilon_+((\exp(-iHt)f,\Omega_-\phi(H_o)P_-\exp(-iHt)f))-$$
$$\varepsilon_+((\exp(-iHt)f,(\Omega_--1)\phi(H_o)P_-\exp(-iHt)f))+$$
$$\varepsilon_+((\exp(-iHt)f,[\phi(H)-\phi(H_o)]\exp(-iHt)f)).$$

In the above, the second, fourth and fifth terms are zero by lemma 3 (iii) while the third is also zero by lemma 3 (iv). As for the first term we note that $(\exp(-iHt)f,\ \Omega_+g)=(\exp(-iH_o t)\Omega_+^* f,g)=0$ since f is orthogonal to the range of Ω_+. This leads to a contradiction unless $F'_+=0$.

The above sketch of the proof shows that the different propagation behaviour for the parts of the phase space with $P.Q>$ or <0 (corresponding to $A \lesseqgtr 0$) plays an essential role. For more than 2-body the general idea persists, however the required partition of the N-body phase space is more complicated.

Next we will say a few words about long-range scattering for 2-body system. In fact this includes one of the most important applications viz the Coulomb potential. Here we face the difficulty early in the game—wave operators as defined before do not exist i.e. the first problem of scattering theory is not well-posed in the form done earlier. We appeal to intuition and see that it is not surprising, for the asymptotic behaviour of the total evolution for such slowly decaying potential is not expected to be that of the free evolution, but as it turns out it is a unitary evolution function of H_o or $\mathbf{P}$.

For any general long-range potential V, it is possible to write $V=V_1+V_2$, where V_1 is the short-range singular part and V_2 is smooth long-range. So without loss of generality we can assume the long-range potential to be smooth and behaving like $|X|^{-\alpha}$ at infinity with $0<\alpha\leqslant 1$. For simplicity, we assume $\alpha>1/2$ (this includes the Coulomb case) and write

$$Y_t=\exp(-iH_o t-iX_t),\quad \text{where } X_t(\mathbf{P})=\int_{t_o}^t V(2s\mathbf{P})\,ds, \tag{6}$$

where t_o is arbitrary, to be suitably chosen.

Then Y_t is an unitary function of momenta and the main theorem is as follows.

Theorem 5: Let V be a smooth long-range potential with $\alpha > 1/2$ and let Y_t be as in (6). Then (i) the modified wave operators (which are isometries) $\Omega_{+} \equiv s-\lim V_t^* Y_t$ as $t \to \pm\infty$ exist and

(ii) the intertwining property holds,

$$H\Omega_{\pm} = \Omega_{\pm} H_o.$$

The detailed proof is long, can be found in (ref. 3) and will not be repeated here. We shall instead observe that (i) implies that the total group V_t asymptotically behaves like Y_t instead of like the free evolution group $\exp(-iH_o t)$, the part X_t providing the distortion. In the case of the Coulomb problem, this is familiar from solution of the stationary Schrodinger equation, and in this case

$$X_t = (4H_o)^{-1/2} \log|t| \, sgn\, t. \qquad (7)$$

The second problem, that of the asymptotic completeness for long-range scattering is very involved and for this we shall only refer to [references 9,10] and to the recent book (Perry)[8].

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